netlognews

NETL's R&D newsletter

July 2009, Issue 14

NETL

U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

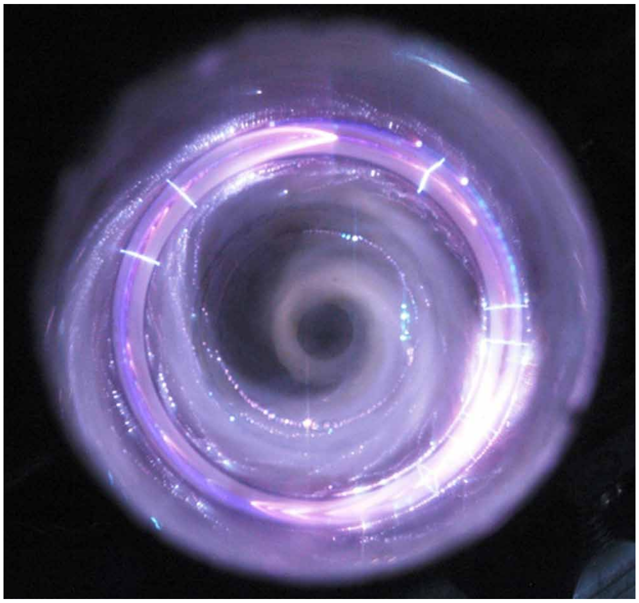
the ENERGY lab

CONTENTS

ON THE COVER

Looking down into a gliding arc vortex plasma reformer.

netlog is a quarterly newsletter, which highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.



Effects of Operating Parameters in Plasma Reformer Quality Studied

NETL researchers are investigating lower-energy plasmas as a means of reforming heavy hydrocarbons – diesel fuel – into hydrogen-rich synthesis gas for use by high-temperature fuel cells being developed in the Solid State Energy Conversion Alliance (SECA) program.

One of the applications is a diesel-fueled auxiliary power unit for long-haul truck transportation.

The researchers conducted runs at Drexel Plasma Institute in a gliding arc vortex plasma reformer to investigate the effects of several key parameters on the liquid hydrocarbon reforming properties.

The NETL researchers used n-tetradecane as a model diesel fuel compound for this study.

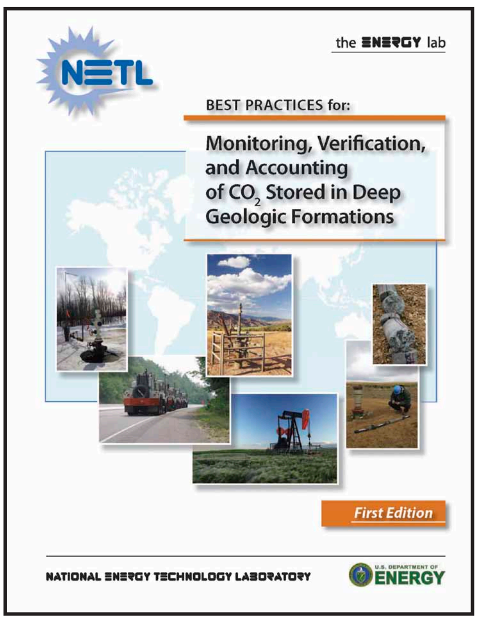
Low temperature non-thermal plasmas are more energy efficient than thermal plasmas. NETL researchers believe the low-temperature plasmas can be a viable alternative to the catalytic process for reforming diesel.

Contact: Dushyant Shekhawat, 304-285-4634

U.S. and U.K. Celebrate Collaboration on Virtual Power Plant Simulation

With a reception at the British Embassy in Washington, DC., researchers and government representatives from the United States and United Kingdom celebrated the successful conclusion of a multi-year collaboration producing compatible, open standards-based software platforms that—with less time, risk and cost—can be applied to represent advanced fossil-energy power generation systems (e.g., gasifiers, combustors, turbines, heat recovery steam generators, and fuel cells). Working under the auspices of a U.S.-U.K. agreement on Collaboration in Energy R&D, the researchers leveraged synergies among the NETL Advanced Process Engineering Co-Simulator, the U.K. Virtual Plant Demonstration Model, and the Computer Aided Process Engineering-OPEN Laboratories Network. The technology was demonstrated by co-simulating the 2,000 MW conventional coal-fired power station located near Didcot in southeast England. The co-simulation enabled process engineers to analyze and optimize overall power plant performance relative to complex fluid flow and thermal phenomena occurring within the furnace.

Contact: Stephen E. Zitney, 304-285-1379



DOE Releases Manual for Safe, Effective Geologic Sequestration

A new US Department of Energy document titled *Best Practices for: Monitoring, Verification, and Accounting of* CO_2 *Stored in Deep Geologic Formations* is now available to regulatory organizations, project developers, national and state policymakers, and interested public. Prepared at NETL with input from the seven Regional Carbon Sequestration Partnerships, the manual provides a comprehensive overview of monitoring, verification, and accounting (MVA) techniques aimed at improving the accuracy of greenhouse gas inventory estimates, and ensuring the safety and efficacy of carbon storage projects. Available technologies can already verify 95 percent retention of sequestered CO_2. The Fossil Energy research and development program expects to demonstrate a suite of technologies capable of ensuring 99 percent retention by 2012.

This document can be accessed via the NETL website.

Contact: Dawn Deel, 304-285-4133

The beaker contains a metal solution used for applying electroplated manganese-cobalt coatings to solid oxide fuel cell interconnect materials.

NETL's Electroplating Process Improves Fuel Cell Performance

An electroplating technique developed by NETL researchers to apply a manganese-cobalt oxide layer on ferritic stainless steel interconnect materials could improve the performance of solid oxide fuel cells.

The research is part of NETL's effort to achieve DOE goals for long-term fuel cell performance research to inhibit degradation of fuel cell interconnect materials.

The first on-cell tests at NETL with manganese-cobalt coated ferritic stainless steel interconnect materials, known as T441, showed that the cell performance degraded by less than 1.5 percent after 600 hours of testing. Cell performance with uncoated T441 interconnect materials degraded about 20 percent during the same test period.

Further optimization of the coating process and investigations of thermal-cycling effects on the interconnect coating are underway.

The new electroplating process offers significant advantages in cost and ease of operations over other coating methods.

This work was conducted in collaboration with Prof. Xingbo Liu's research group at West Virginia University under the University Research Initiative program.

Contact: Randy Gemmen, 304-285-4536

New Concept Integrates CO_2 Cycle from Generation to Deposition

Having found that the CO_2 adsorption capacity of certain overburden materials is comparable to that of coal, NETL researchers conceived a novel carbon sequestration approach using waste materials generated during coal production. If power generation were co-located with coal extraction/preparation, carbon capture could be facilitated by a controlled sequential heating and cooling of these solids with the exhaust heat of combustion.

This method avoids logistical problems and potentially significant transportation costs of delivering captured CO_2 from a power generation station to a remote sequestration site. It also avoids limitations associated with carbon sequestration in unmineable seams of coals that have shown a propensity to swell as the coal matrix imbibes CO_2.

A feature *article* entitled, "CO_2 Storage in Shallow Underground and Surface Coal Mines: Challenges and Opportunities," in the American Chemical Society publication *Environmental Science & Technology* (Vol. 43, No. 3, pg. 561ff.) describes the approach.

Contact: Vyacheslav Romanov, 412-386-5476

Bob Stevens and Ranjani Siriwardane (holding the patented sorbent) standing in front of the reactor system where the sorbent is being tested.

Novel Regenerable Sorbent Developed for CO_2 Capture

NETL researchers are studying a novel sorbent invented at NETL with high capacity for capturing carbon dioxide (CO_2).

The sorbent, consisting of magnesium hydroxide, was developed for CO_2 capture at 200–315 °C. It is suitable for CO_2 capture applications such as coal gasification systems. This is a unique warm gas temperature CO_2 removal sorbent since the regeneration temperature is significantly lower than previously reported.

Both experimental data and thermodynamic analysis data showed that the sorbent is regenerable at 375 °C at high pressure and that steam does not affect the sorbent performance. A multi-cycle test conducted in the high pressure fixed-bed flow reactor at 200 °C with 28 percent CO_2 showed stable reactivity during the cyclic tests. The capture capacity also increased with increasing pressure.

The sorbent is unique since it possesses a high CO_2 capture capacity of more than 3 moles/kg at 200 °C as well as being regenerable at a low temperature of 375 °C and high pressure. High pressure regeneration is advantageous since the CO_2 compression cost required for sequestration can be reduced. NETL has received a U.S. patent for this research.

A paper about the study was accepted for publication in *Industrial & Engineering Chemistry Journal.* The paper is entitled, "Novel Regenerable Magnesium Hydroxide Sorbents for CO_2 Capture at Warm Gas Temperatures."

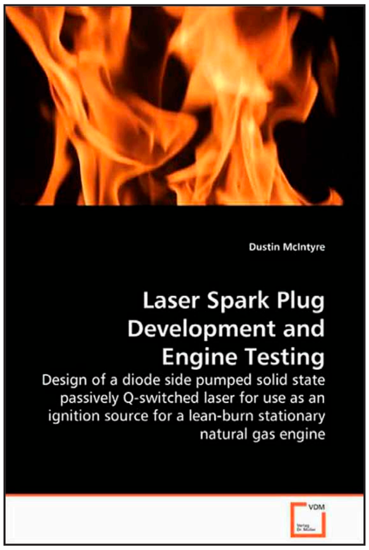
Contact: Ranjani Siriwardane, 304-285-4513

Article Describes Interactions of Jet Fuels with Nitrile Rubber O-Rings

An article recently published in *Energy & Fuels* (2009, 23, 857-861) describes how a transition from petroleum-derived to synthetic Fischer-Tropsch jet fuels may affect the leaching of plasticizers from nitrile o-rings used in jet fuel systems. Research showed that many of the plasticizer and stabilizer compounds were removed from the o-rings regardless of the contact fuel. Fuel molecules were observed to migrate into the o rings for the petroleum-derived fuel as did both the fuel and additive for a synthetic F-T jet fuel additized with benzyl alcohol, but less for the unadditized synthetic fuel.

The specific compounds or classes of compounds involved in the partitioning were identified and a semiquantitative comparison of relative partitioning of the compounds of interest was made. These results provide another step forward in improving the confidence level of using additized, fully synthetic jet fuel in the place of petroleum-derived fuel. The *paper* entitled, "Interactions of Jet Fuels with Nitrile O-Rings: Petroleum-Derived Versus Synthetic Fuels," was authored by Robert Gormley et al.

Contact: Robert Gormley, 412-386-5957



Doctoral Dissertation on Miniaturized Laser Spark Plug Design Published

A German publishing company has published a book by NETL researcher Dustin McIntyre, which is the formal publication of his doctoral dissertation on research performed at NETL's reciprocating engine laboratory. The book outlines the design of a miniaturized laser spark plug used to enable the operation of large bore natural gas engines at higher efficiencies and leaner conditions. The spark plug was designed to replace traditional electrical spark plugs that quickly wear out at the modified engine conditions where the higher efficiencies are achievable. The work was sponsored by EERE's Advanced Reciprocating Engines Program from 2002 to 2007. The title of the book is "Laser Spark Plug Development and Engine Testing: Design of a diode side pumped solid state passively Q switched laser for use as an ignition source for a lean-burn stationary natural gas engine," ISBN 978-3-639-11362-4.

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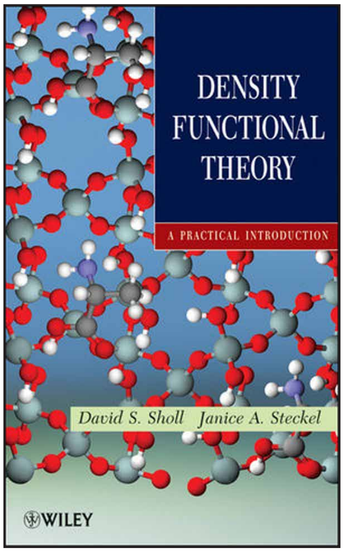


Computational Scientist Coauthors Book on Density Functional Theory

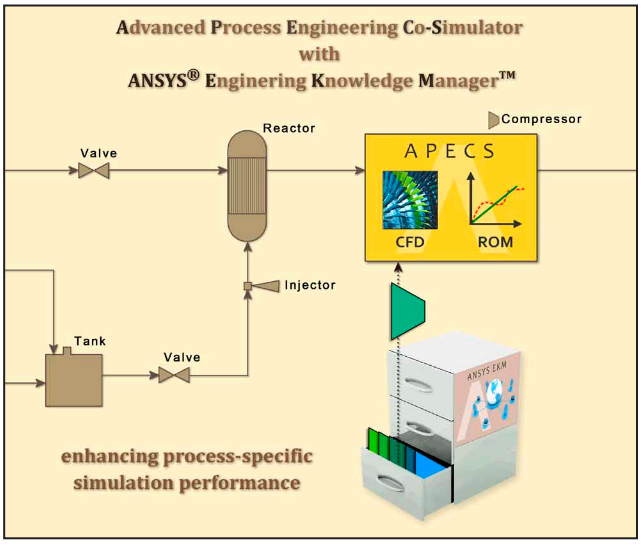
NETL physical scientist Dr. Janice A. Steckel has published a book about density functional theory calculations.

Density functional theory, or DFT, is an important tool used for making predictions about the properties of molecules, solids and surfaces as well as for giving quantitative and qualitative predictions about chemical reactions. This book was written to provide a readable introduction for students, theorists and/or experimentalists interested in performing their own DFT calculations. Examples and exercises are included, as well as extensive references for further reading.

The aim of the book is not to present the theoretical derivation of the equations that are solved in typical DFT calculations, but rather to provide a practical guide that can be used by persons from diverse backgrounds.

"A Practical Introduction to Density Functional Theory Calculations" is coauthored by Dr. David S. Sholl, a professor of chemical and biomolecular engineering at the Georgia Institute of Technology and was published by John Wiley & Sons, Inc., ISBN: 978-0-470-37317-0.

Contact: Janice Steckel, 412-386-4430



New Version of NETL's APECS Software (Version 1.6) Released

The R&D 100 award-winning Advanced Process Engineering Co-Simulator (APECS) with ANSYS® Engineering Knowledge Manager™ (EKM™), Version 1.6, offers several important enhancements for efficiently solving process/equipment co-simulations arising from large-scale energy applications such as IGCC systems.

If a parallelized computational fluid dynamics (CFD) solver (e.g., FLUENT®) is available for a given equipment model (e.g., gasifier), it can be executed on multiple processors to reduce turnaround time. For co-simulations involving two or more CFD-based equipment models (e.g., gasifier and gas turbine combustor), the APECS "super" block feature provides the ability to run multiple CFD models in parallel to converge the overall process simulation (e.g., IGCC).

APECS v1.6 also provides a fast reduced order model (ROM) solver based on coupling an artificial neural network (ANN) for nonlinear regression with principal component analysis (PCA) for generating the flow field and other contours. In a gas turbine combustor case study, the ANN/PCA-based ROM not only reduced computational time by several orders of magnitude, but also predicted combustor outlet temperatures with less than 3.0 percent error when compared to results from the high-fidelity CFD model.

By providing solutions on both ends of the performance spectrum, including parallel execution of the CFD models on high-performance computers and the use of fast ROMs based on CFD results, APECS v1.6 addresses the performance issue that equipment simulations based on high-fidelity CFD models require much more computational time than equipment simulations based on simplified engineering models, especially for cases in which one or more CFD models are embedded in large-scale energy system co-simulations.

The APECS with EKM™ software was developed by a collaborative team including NETL, ANSYS, Aspen Technology, ALSTOM Power, Carnegie Mellon University, and Iowa State University. This software suite was recently highlighted at the AspenTech's 2009 worldwide user conference.

Contact: Stephen E. Zitney, 304-285-1379

Computationally Efficient Modeling Technique Applied to Power Plant Equipment

Participants in the NETL Collaboratory for Process and Dynamic Systems Research have developed a new algorithm for reduced order modeling (ROM) that speeds-up the detailed analysis and optimization attainable with computational fluid dynamics (CFD) when performing process co-simulation. Separate case studies involving the use of comprehensive CFD models for two power plant equipment items, namely a gas turbine combustor and an entrained-flow coal gasifier, show that the new ROM methodology based on principal component analysis is both effective and efficient, and suitable for incorporation as an option in NETL's award-winning Advanced Process Engineering Co-Simulator (APECS). These studies, including theoretical development, are described in the American Chemical Society journal, *Energy & Fuels* (Vol. 23, No. 3, pg. 1695ff.).

Contact: Stephen E. Zitney, 304-285-1379

Miami University of Ohio Receives Research Assistance

Thomas D. Brown, a senior research engineer, provided final design concepts and practical techniques of operation for a methane or natural gas hydrate (NGH) formation and dissociation facility at Miami University of Ohio (MUO) in Oxford, Ohio. Professors and students at MUO have been involved in a collaborative research effort over the past year with NETL researchers to investigate rapid formation of methane or natural gas hydrates in cooperation with Parsons.

These R&D efforts are focused on the further development of economic natural gas storage and transport techniques. NETL provided a 1-liter autoclave, design approaches and reviews, with MUO students building the facility which is designed to focus on the impact of heat released during water super cooling phase prior to natural gas hydrate formation. The rate at which heat is being released could aid or hinder hydrate formation (especially hindering during atypical rapid formation investigations).

Brown spent four days at MUO working with the professors and students, assisting them with the final assembly and operation of the autoclave. In subsequent weeks following Brown's visit MUO undergraduate students, through their efforts on this senior year project/facility, earned an A in the associated course. This type of research study is normally performed at a graduate level.

Contact: Thomas D. Brown, 412 386 4691

NETL and Pitt Collaborate to Build World's Only Aerothermal Test Rig of its Kind

A collaborative team of researchers from NETL and University of Pittsburgh has completed design and construction of an aerothermal test rig capable of using superheated steam and/or CO_2 as the working fluid.

There is no other such facility in the global energy research community.

Technical information generated from this test rig will directly benefit the advancement of cooling technology for our nation's future fossil power generation systems, especially for those based on oxy-fuel cycles with turbine inlet temperature reaching the unprecedented level of 1750°C.

The rig has been through shakedown testing and is being used to explore the heat transfer performance of advanced vortex generators in internal cooling passages for turbine airfoils.

Contact: Mary Anne Alvin, 412-386-5498

Atomic Structure of Fischer-Tropsch Catalysts Study Published

Researchers in NETL's Chemistry and Surface Science Division have published a study that provides detailed images of the atomistic structure of iron oxide catalysts similar to those used for converting gasified coal into liquids that can be used as hydrogen carriers or fuels. This work appeared in the highly-regarded, peer-reviewed, publication, Journal of Physical Chemistry C. The manuscript investigates the production of model iron and iron oxide catalyst particles on an inert gold growth substrate. Researchers characterized the atomic-scale structure of the particles using advanced surface analysis techniques, such as scanning tunneling microscopy. These particles serve as model catalysts reproducing the size, shape, defects, and other important structural features of real world iron-based catalysts used for the Fischer-Tropsch process.

Future work will focus on incorporating promoters, such as copper, into this system to better understand the mechanism involved in activating Fischer-Tropsch catalysts.

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